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High Order Symplectic Integration Methods for Finite Element Solutions to Time Dependent Maxwell Equations

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www.llnl.gov/casc/emsolve

Maxwell's Equations: Continuum and Discrete

We begin with the coupled first order Maxwell equations, then discretize in space via a Galerkin Finite Element Method to yield a linear system of ODEs:

$$e\frac{\partial}{\partial t}\vec{E} = \nabla \times \left(m^{-1}\vec{B}\right) - \vec{J}(t) \qquad \mathbf{M}_e \frac{\partial}{\partial t}\mathbf{e} = \mathbf{K}^T\left(\mathbf{M}_m \mathbf{b}\right) - \mathbf{M}_e \mathbf{j}$$

$$\frac{\partial}{\partial t}\vec{B} = -\nabla \times \vec{E} \qquad \frac{\partial}{\partial t}\mathbf{b} = -\mathbf{K}\ \mathbf{e}$$

We use discrete differential form basis functions of arbitrary polynomial degree:

$$\mathbf{M}_e[i,j] = \int_\Omega (e\vec{w}_i)\cdot(\vec{w}_j), \quad \vec{w}_i \in W_h \subset H(Curl)$$

$$\mathbf{M}_m[i,j] = \int_\Omega (m^{-1}\vec{f}_i)\cdot(\vec{f}_j), \quad \vec{f}_i \in F_h \subset H(Div)$$

$$\mathbf{K}[i,j] = A_i(\nabla \times \vec{w}_j)$$

i.e. the projection of the curl of a 1-form onto the discrete 2-form space

Second Order Accurate Leap Frog Method

Consider the very popular second order accurate "Leap-Frog" method applied to the system of ODEs (ignoring the current source):

$$\frac{\partial}{\partial t}\mathbf{e} \approx \frac{\mathbf{e}_{n+1} - \mathbf{e}_n}{\Delta t}$$

$$\frac{\partial}{\partial t}\mathbf{b} \approx \frac{\mathbf{b}_{n+1} - \mathbf{b}_n}{\Delta t}$$

$$\longrightarrow$$

$$\mathbf{e}_{n+1} = \mathbf{e}_n + \Delta t \mathbf{M}_e^{-1}\mathbf{K}^T\mathbf{M}_m\mathbf{b}_n$$

$$\mathbf{b}_{n+1} = \mathbf{b}_n - \Delta t \mathbf{K}\mathbf{e}_{n+1}$$

This explicit method is well known to be

energy conserving and ***conditionally stable***

Given the high order accuracy of our compatible spatial discretization method, can we apply high order accurate time integration methods to the discrete Maxwell equations that are still energy conserving and conditionally stable?

Symplectic Time Integration

Consider the case of a simple undamped harmonic oscillator:

Harmonic Oscillator

$$\dot{p} = q$$

$$\dot{q} = -p$$

$$p^2 + q^2 = 1$$

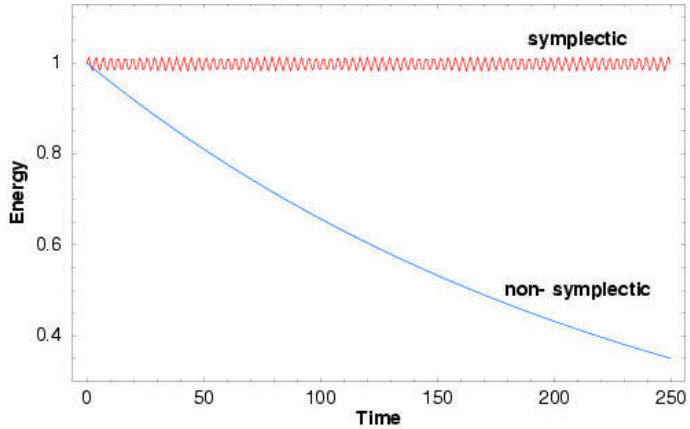
Spatially-Discrete Maxwell

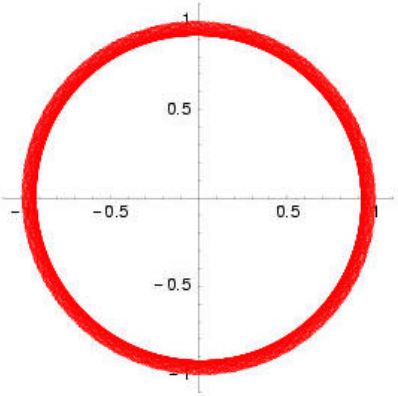
$$\dot{\mathbf{e}} = \tilde{\mathbf{C}}\mathbf{b}$$

$$\dot{\mathbf{b}} = -\mathbf{C}\mathbf{e}$$

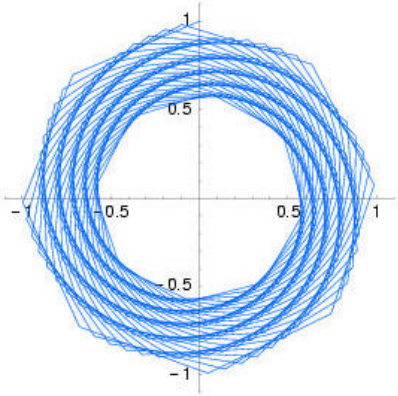
$$\mathbf{e}^T\mathbf{M}_e\mathbf{e} + \mathbf{b}^T\mathbf{M}_m\mathbf{b} = \text{constant}$$

Traditional integration methods (such as Runge-Kutta) introduce numerical dissipation. Higher order accurate and non-dissipative symplectic methods have been developed for Hamiltonian systems with applications in astrophysics and molecular dynamics.





Symplectic Method



Non-Symplectic RK Method

General Symplectic Integration Algorithm

$$
\begin{aligned}
&\textbf{for } i = 1 \textbf{ to } nstep \textbf{ do:} \\
&\quad \mathbf{e}_{in} = \mathbf{e}_i \\
&\quad \mathbf{b}_{in} = \mathbf{b}_i \\
&\quad \textbf{for } j = 1 \textbf{ to } order \textbf{ do:} \\
&\qquad t_j = i\Delta t + \sum_{n=1}^{j-1} a_n \Delta t \\
&\qquad \mathbf{e}_{out} = \mathbf{e}_{in} + b_j \Delta t \mathbf{M}_e^{-1} \mathbf{K}^T \mathbf{M}_m \mathbf{b}_{in} \\
&\qquad \mathbf{b}_{out} = \mathbf{b}_{in} - a_j \Delta t \mathbf{K} \mathbf{e}_{out} \\
&\quad \textbf{end} \\
&\quad \mathbf{e}_{i+1} = \mathbf{e}_{out} \\
&\quad \mathbf{b}_{i+1} = \mathbf{b}_{out} \\
&\textbf{end}
\end{aligned}
$$

Coefficients for symplectic integration methods of order *1* through *4* have been derived*. Note that the leap-frog method corresponds to the first order case.

**Forest & Ruth '90, Candy & Rozmus '91*

Order 1 – Truncation Error = Δt^2	
$\alpha_1 = 1$	$\beta_1 = 1$
Order 2 – Truncation Error = Δt^3	
$\alpha_1 = 1/2$	$\beta_1 = 0$
$\alpha_2 = 1/2$	$\beta_2 = 1$
Order 3 – Truncation Error = Δt^4	
$\alpha_1 = 2/3$	$\beta_1 = 7/24$
$\alpha_2 = -2/3$	$\beta_2 = 3/4$
$\alpha_3 = 1$	$\beta_3 = -1/24$
Order 4 – Truncation Error = Δt^5	
$\alpha_1 = (2 + 2^{1/3} + 2^{-1/3})/6$	$\beta_1 = 0$
$\alpha_2 = (1 - 2^{1/3} - 2^{-1/3})/6$	$\beta_2 = 1/(2 - 2^{1/3})$
$\alpha_3 = (1 - 2^{1/3} - 2^{-1/3})/6$	$\beta_3 = 1/(1 - 2^{2/3})$
$\alpha_4 = (2 + 2^{1/3} + 2^{-1/3})/6$	$\beta_4 = 1/(2 - 2^{1/3})$

High Order Update Scheme and Numerical Stability

The generalized k^{th} order symplectic update method applied to the discrete Maxwell equations can be written as a product of amplification matrices:

$$\begin{bmatrix} \mathbf{e}_{n+1} \\ \mathbf{b}_{n+1} \end{bmatrix} = \left(\prod_{i=1}^{k} \mathbf{Q}_i \right) \begin{bmatrix} \mathbf{e}_n \\ \mathbf{b}_n \end{bmatrix}$$

$$\mathbf{Q}_i = \begin{bmatrix} \mathbf{I} & b_i \Delta t \mathbf{M}_e^{-1} \mathbf{K}^T \mathbf{M}_m \\ -a_i \Delta t \mathbf{K} & \mathbf{I} - a_i b_i \Delta t^2 \mathbf{K} \mathbf{M}_e^{-1} \mathbf{K}^T \mathbf{M}_m \end{bmatrix}$$

A necessary condition for stability is then:

$$r(\mathbf{Q}_i) \le 1 \quad \longrightarrow \quad \Delta t \le \frac{2}{\sqrt{r(a_i b_i \mathbf{K} \mathbf{M}_e^{-1} \mathbf{K}^T \mathbf{M}_m)}}$$

Numerical Stability (cont.)

Now consider the similar amplification matrix:

$$\tilde{\mathbf{Q}}_i = \begin{bmatrix} \mathbf{I} - a_i b_i \mathbf{A}\mathbf{A}^T & -a_i \mathbf{A} \\ b_i \mathbf{A}^T & \mathbf{I} \end{bmatrix}$$

In order for $r(\mathbf{Q}_i) \le 1$ to be a **sufficient** condition for stability, we need to exhibit $n_1 + n_2$ linearly independent eigenvectors of $\tilde{\mathbf{Q}}_i$, where $n_1 = Dim(\mathbf{e})$ and $n_2 = Dim(\mathbf{b})$

Suppose:

1) $Rank(\mathbf{A}) = m$

2) The eigenvalues m of $a_i b_i \mathbf{A}\mathbf{A}^T$ satisfy $0 \le |m| \le 2$

Numerical Stability (cont.)

Then:

Conservation of Numerical Energy:

1) The eigenvalues of $\tilde{\mathbf{Q}}_i$ lie on the unit circle

Numerical Stability:

2) The eigenvectors of $\tilde{\mathbf{Q}}_i$ form an eigenbasis in $R^{n_1+n_2}$

Proof:

By analyzing the eigenvalues and eigenvectors of: $a_i b_i \mathbf{A}\mathbf{A}^T \mathbf{x} = l\,\mathbf{x}$

and since $Dim(Null(\mathbf{A})) = n_1 - m$ and $Dim(Null(\mathbf{A}^T)) = n_2 - m$

we can generate $2m + (n_1 - m) + (n_2 - m) = n_1 + n_2$

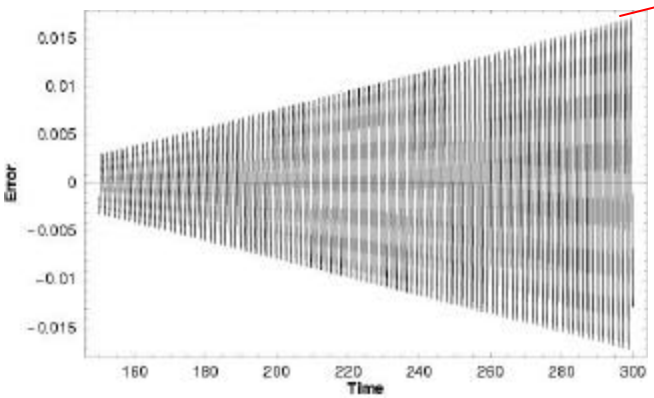
linearly independent eigenvectors of the amplification matrix $\tilde{\mathbf{Q}}_i$

Higher Order Time Integration: Global Phase and Energy Error

- ***1st Order Method:***
- **Time Step** = 0.005 sec
- **# Steps** = 60,000
- **CPU time / step** = 0.0941 sec
- **Total Run Time** = 94.1min

- ***3rd Order Method:***
- **Time Step** = 0.015 sec
- **# Steps** = 20,000
- **CPU time / step** = 0.2976 sec
- **Total Run Time** = 99.2 min

.015



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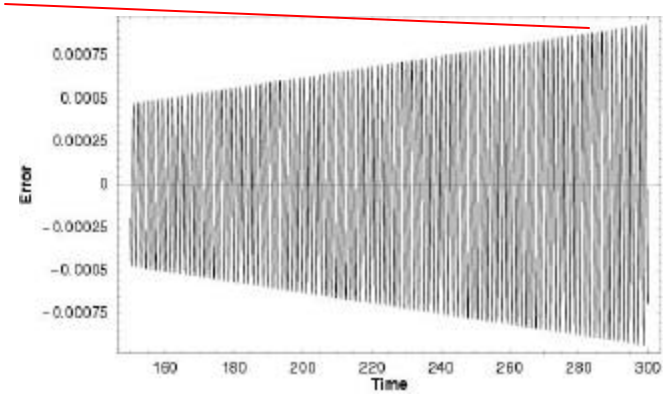
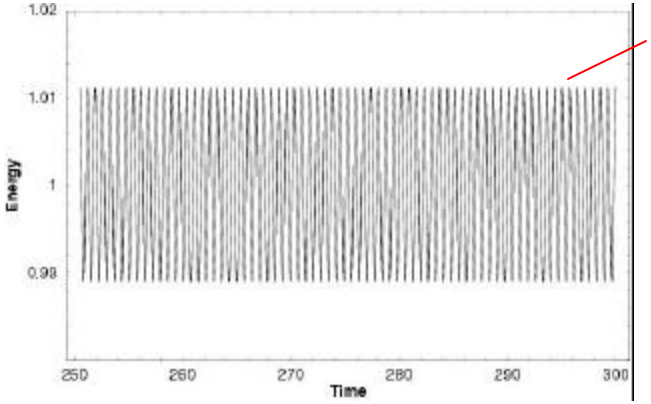


20x More Effective!

1.01



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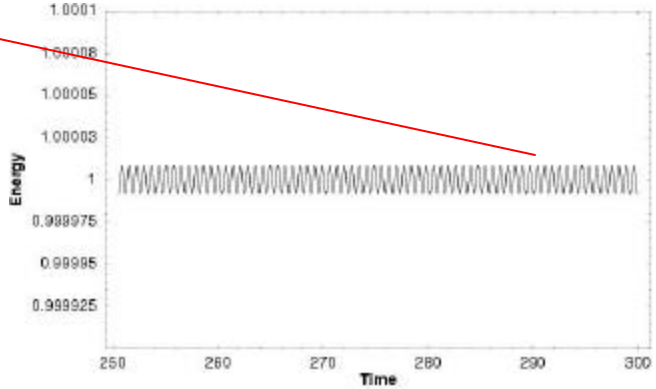
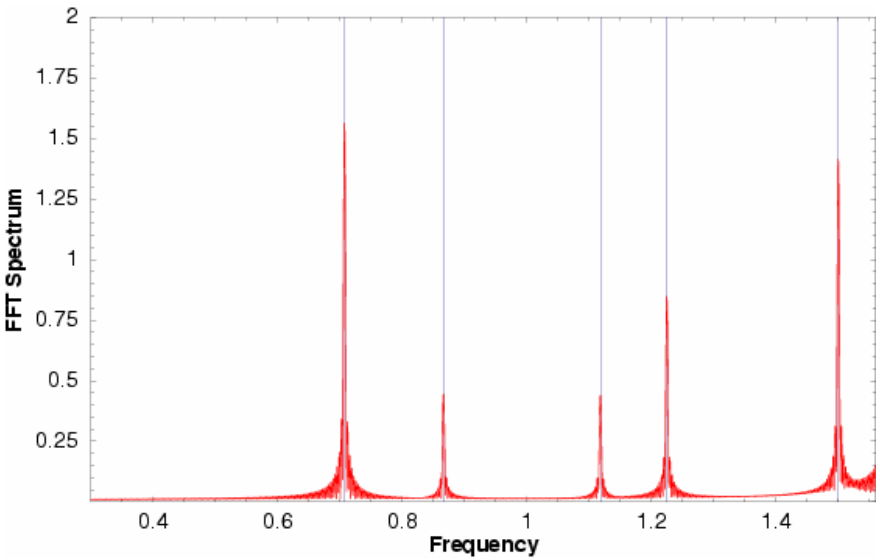


Resonant Cavity Analysis

Here we compute the resonant modes of a cubic cavity using two different integration methods in conjunction with a high order ($p = 4$) compatible spatial discretization. Use of high order in both time and space is required to achieve maximal accuracy.



	1st Order	3rd Order
Physical Time	300 sec	300 sec
Time Step	0.005 sec	0.015 sec
No. Steps	60,000	20,000
Avg CPU time/step	0.0941 sec	0.2976 sec
Total Run Time	94.1 min	99.2 min
Error in 1st Mode	1.3809e-3	1.0935e-4
Error in 2nd Mode	8.9125e-4	3.8032e-4
Error in 3rd Mode	5.3780e-4	5.3780e-4
Error in 4th Mode	1.5442e-3	2.7264e-4
Error in 5th Mode	3.2044e-3	6.1035e-4

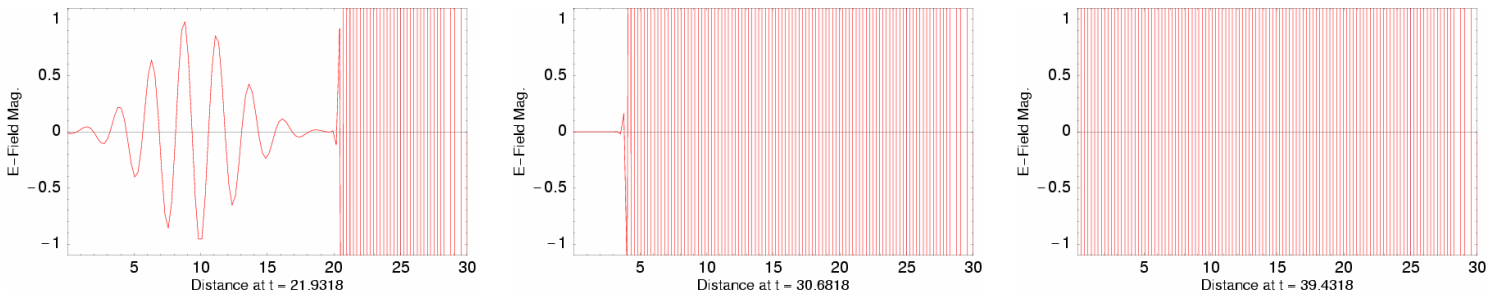
Conductivity Terms and Implicit Time Stepping

In order to introduce conductivity terms while still maintaining numerical stability, we can treat the problem implicitly:

$$(1+\frac{\Delta t}{2}\mathbf{M}_e^{-1}\mathbf{M}_s)\mathbf{e}_{n+1} = (1-\frac{\Delta t}{2}\mathbf{M}_e^{-1}\mathbf{M}_s)\mathbf{e}_n + \Delta t\mathbf{M}_e^{-1}\mathbf{K}^T\mathbf{M}_m\mathbf{b}_n$$

$$(1+\frac{\Delta t}{2}\mathbf{M}_{s*})\mathbf{b}_{n+1} = (1-\frac{\Delta t}{2}\mathbf{M}_{s*})\mathbf{b}_n - \Delta t\mathbf{K}\mathbf{e}_{n+1}$$

Explicit 4th Order Symplectic:



Implicit 4th Order Symplectic: